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Quantum-chemical Study of the Structure and Reactivity of Pyrazol-5-ones and Their Thio and Seleno Analogs. III. Semiempirical Calculations of the Structure and Acid-Base Properties of 1-Methyl-4H-pyrazol-5-one, -thione, and -selenone

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Abstract

Tautomerism and acid-base properties of 1-methyl-4H-pyrazol-5-one and its thio and seleno analogs were studied by the semiempirical quantum-chemical methods MNDO, AM1, and PM3. The CH form prevails in pyrazolone, whereas the EH forms (E = S, Se) prevail in heteroanalogs. The calculations predict an increase in the gas-phase acidity in the series O < S < Se. The gas-phase basicity of these compounds does not change in such a regular manner.